

Nonylphenyl diphenyl phosphate, mixed isomers
64532-97-4 | DTXSID4025797

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

Model Results

Predicted value: 54500 L/kg

Global applicability domain: Outside

Local applicability domain index: 3.71e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|--|
| <div>Image not found</div> <div>Fluvalinate</div> <div>Measured: 507000</div> <div>Predicted: 293000</div> | <div>Image not found</div> <div>tau-Fluvalinate</div> <div>Measured: 507000</div> <div>Predicted: 284000</div> | <div>Image not found</div> <div>Nonylphenyl diphenyl phosphate, mixed isomers</div> <div>Measured: 11500</div> <div>Predicted: 54500</div> |
| <div>Image not found</div> <div>Flucythrinate</div> <div>Measured: 100000</div> <div>Predicted: 155000</div> | <div>Image not found</div> <div>Bis(2-ethylhexyl) terephthalate</div> <div>Measured: 14500</div> <div>Predicted: 12500</div> | <div>Image not found</div> <div>Dioctyl phthalate</div> <div>Measured: 24000</div> <div>Predicted: 17100</div> |